Propylene glycol diacetate

623-84-7 | DTXSID9044827

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -23.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.72e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

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Diethyl propanedioate
Measured: -50.0
Predicted: -34.4

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Dimethyl glutarate
Measured: -42.5
Predicted: -25.9

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Diethyl butanedioate
Measured: -21.0
Predicted: -13.4

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Dimethyl adipate
Measured: 10.3
Predicted: -9.04